Future Trends in Applied & Computational Mathematics for Defense Applications

Anna Tsao
Defense Sciences Office

1

I am here today to try to influence future trends in the application of mathematics by you, the DoD community, because I believe that we have within our grasp quantum leaps in the DoD's ability to fulfill its mission. During the last ten years, through the innovations in computer science and engineering, there have been dramatic improvements in speed of computational platforms available. What is only beginning to be realized is that without fast algorithms that overcome the curse of dimensionality, all this computational power is of limited value.

Over the last ten years a number of extraordinary algorithms have been developed that owe their superior characteristics to mathematical representations chosen in an appropriate physically motivated waveform domain. Such representations, based on a mathematical field known as harmonic analysis, have led to breakthroughs in conquering two of the main sources of high dimensionality, namely, computational complexity and degrees of freedom in data. This mathematical machinery has now been demonstrated sufficiently many times in different contexts that a compelling case can be made that this powerful set of methods is broadly applicable and will have a pervasive and lasting impact on computational science and on DoD applications. I would like to highlight two important areas where high payoffs appear indicated if all-out assaults are made.

What's Lurking Over the Horizon?

- Well-conditioned fast (near-linear complexity) algorithms for analysis and simulation of physical phenomena:
  - Electronic device and antenna field simulation.
  - Computational quantum mechanics.
  - Modeling biomolecular interactions.
  - Navier-Stokes solutions.
- Rapid, effective exploitation of high-dimensional data:
  - Bioactivity prediction from molecular structure.
  - Strategic/tactical planning from digital maps and imagery.

2

The first impact area is in the development of what I will call well-conditioned fast algorithms. I will give examples where accurate, near-linear complexity algorithms have been developed for analyzing and/or simulating a broad spectrum of physical phenomena on scales that would not be possible otherwise, even given optimistic assumptions regarding hardware. The methods all use mathematical representations that derive their efficacy from the fact that they are well-matched to the underlying physical phenomena. I will try to highlight the main reasons why the mathematical machinery being developed is so revolutionary. I list here some of the notable problem areas where these methods are expected to provide big future payoffs, some of which might be surprising to you.

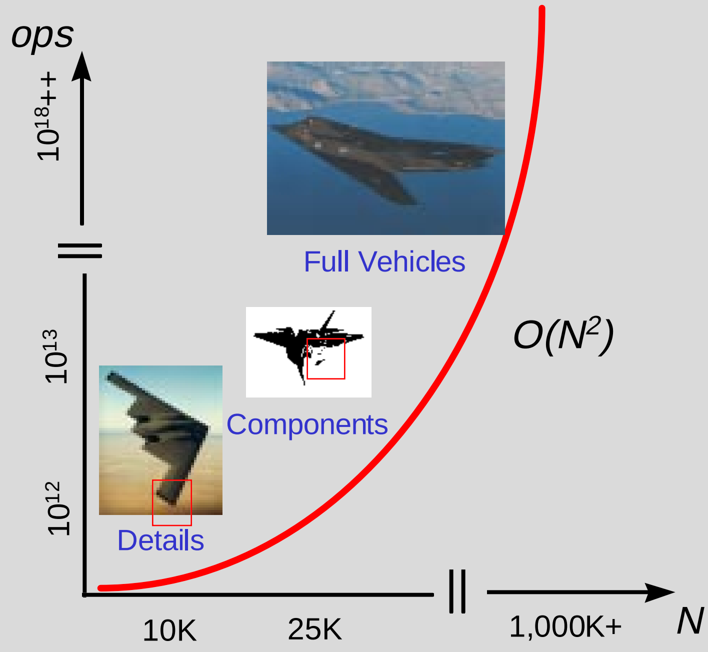
The second critical impact area I will discuss is in the exploitation of high-dimensional data, i.e., data with a high number of degrees of freedom. The main issue in such applications is the ability to mathematically represent the data to allow searches to be performed in spaces where the number of degrees of freedom is low. As will be illustrated, the same paradigm of matching representation to the underlying physical phenomena is invaluable to successful data exploitation. Important data exploitation challenges confront us in virtually all applications, including the prediction of function from structure for use in biological warfare defense and the exploitation of large and diverse map and imagery databases for military planning.

Well-Conditioned Fast Algorithms

3

Method of Moments

- 20K on supercomputers.
- 100K+ on superduper computers.
- 1,000K+: ***no way!***
- Can't ensure accuracy.
- Complicated meshing schemes required.



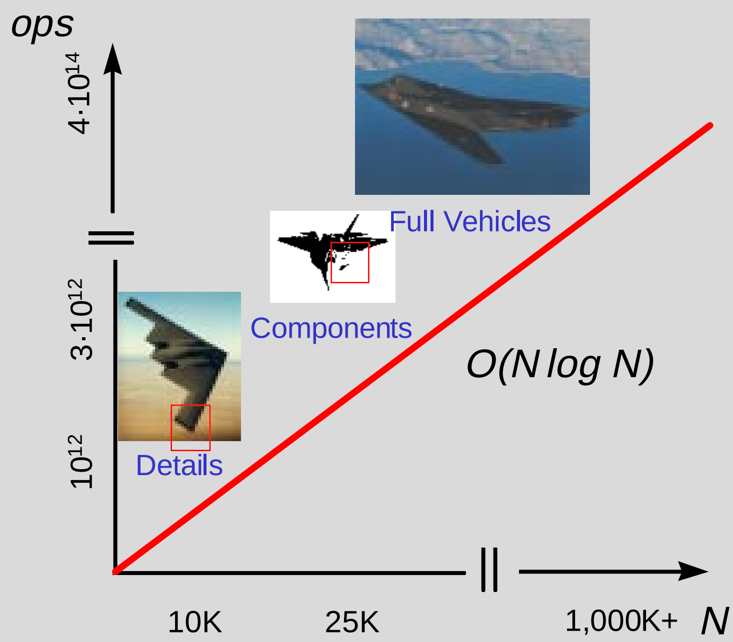
4

The first example is the most spectacular to date that can be reported. The radar cross section (RCS) of bodies that are very large relative to a wavelength, but whose surfaces have small-scale features which cannot be resolved by high frequency asymptotic techniques, has historically been calculated by the frequency domain method of moments (MoM), which scales as N^2. The size of the matrix, N, is proportional to the surface area of the object being modeled and is typically on the order of 1,000,000 or more for full-size aircraft. Hence, RCS calculations using MoM can be applied only to relatively small components of extended objects, even on supercomputers. In addition, such methods are severely limited by an inability to ensure accuracy and the need for complicated mesh generation schemes.

Fast Multipole Method

DARPA

- 20K on desktops.
- 100K+ on servers.
- 1,000K+ on supercomputers.
- Prescribable accuracy for low additional cost.
- No complex mesh generation procedures required.

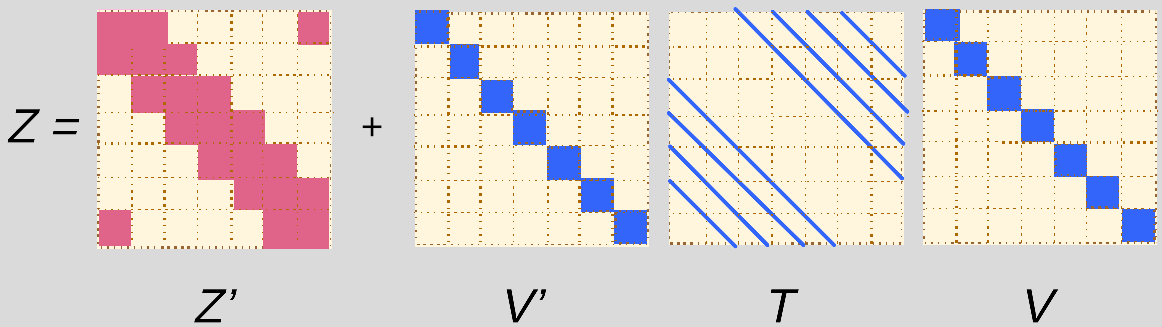


5

In contrast, the Fast Multipole Method (FMM) will allow the routine calculation of electromagnetic scattering off of full-scale aircraft and missiles at high frequencies with prescribable accuracy and dramatically simplified discretization requirements. Currently, problems are being solved on high-end workstations by Boeing and others that previously required massively parallel computing capability.

Sparse Decomposition of Z

Integral equation formulation reduces to solving dense linear $N \times N$ system $ZI = V$, where N scales as surface area. Z has sparse decomposition:



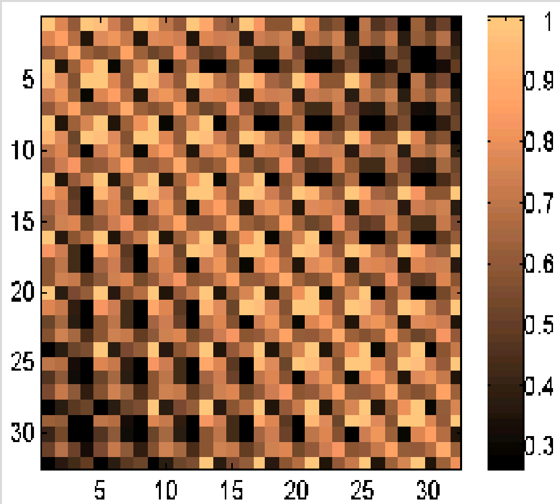
Results in O(N log N) vs. $O(N^2)$ algorithm and substantial memory savings!

6

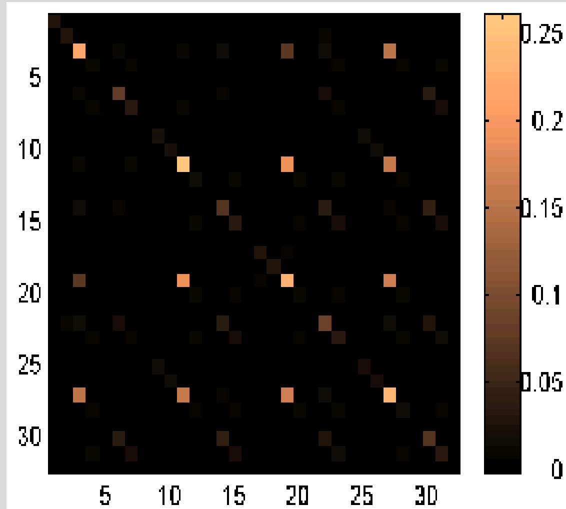
The RCS is computed by discretizing an integral equation, leading to a dense linear system ZI = V. Solving this N x N dense system iteratively, as is usually done to minimize computation, requires O(N2) operations, since the matrix Z is applied to successive approximations of the desired vector I until convergence occurs. Z can be regarded as the matrix of interactions amongst N scatterers. FMM achieves a reduction in the cost of computing and applying Z by using a mathematical formulation that sub-blocks Z into groups of scatterers and exploits the fact that the physics allows treating the near- and far-field interactions separately. This formulation results in remarkably sparse matrices.

In the near-field, interactions must all be computed directly, leading to a banded matrix. However, in the far field, it turns out that because scattering just behaves like a collection of plane waves, there is a block diagonal operator that simultaneously diagonalizes all far field interaction submatrices! Recursively applying this scheme in a hierarchical fashion at successively finer scales leads to an O(N log N) algorithm. Furthermore, in contrast to previous methods, a suitably chosen combined field integral equation formulation leads to a well-conditioned matrix system, resulting in prescribable accuracy in the computed solutions. Use of high order methods allows significant matrix size reductions and additional digits of accuracy to be achieved with low additional cost. Finally, the well-conditioned formulation, combined with the use of quadrature formulae, greatly simplifies the discretization requirements to a sampling density issue on the surface, compared to the usual complicated scheme requiring a combination of interpolation on facets, as well as aspect ratio control.

Space Time Adaptive Processing - I



Covariance matrix
(Monostatic ground clutter)

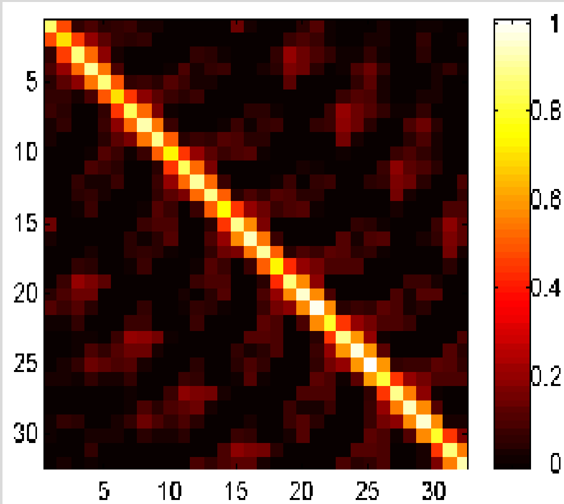


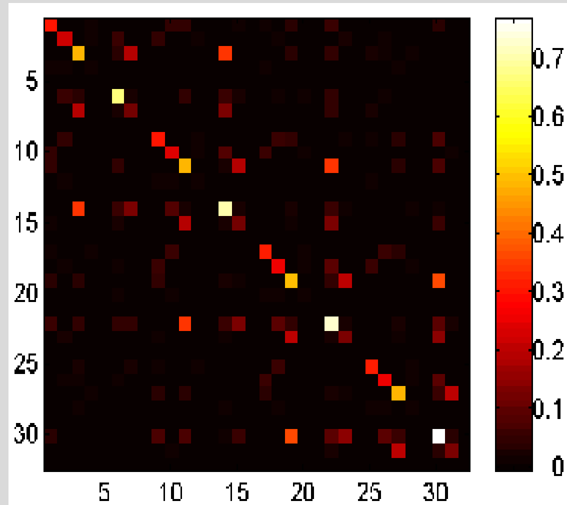
Wavelet Block Filtered Rearranged Covariance Matrix

7

In this example, we illustrate the ability of adapted waveforms such as wavelets to efficiently represent coherence in physical phenomena. The matrix on the left is a space time covariance matrix for data representative of monostatic ground clutter in the main beam of a missile antenna. On the right is the matrix that has been compressed using wavelets after a physically appropriate rearrangement of elements. This compression confirms that there is little information in the return.

Space Time Adaptive Processing - II





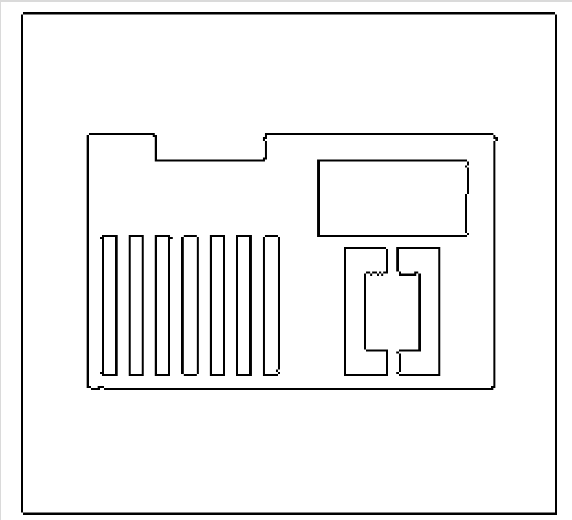
Covariance matrix (Wideband jamming interference)

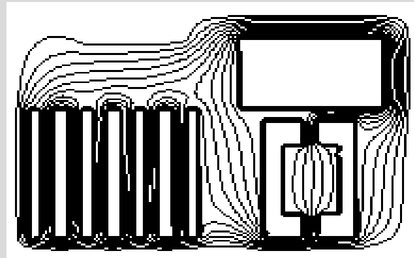
Wavelet Block Filtered Rearranged Covariance Matrix

8

This example illustrates similar compression methods applied to wideband jamming interference covariance matrices. In this case, the left hand matrix is the space time covariance matrix for a single Pulse Repetition Interval (PRI) using 4 channels and 8 time taps. The compression algorithm was designed to take advantage of the block structure of the covariance matrix. Ninety percent of the resulting matrix elements are less than 1% of the maximum matrix element. Furthermore, preliminary work indicates that meaningful compression is possible without loss of signal to noise. The resulting matrix is certainly not as highly compressed as in the previous slide, but nonetheless indicates the strong potential for significant reductions in the processing required by the missile in seeking its target, assuming appropriate algorithms for processing the compressed matrix can be constructed.

Fast Poisson Solvers





- Only few times greater cost than standard solver on a uniform rectangular mesh.
- Prescribable accuracy for low additional cost.
- Does not require complex mesh generation procedures.

9

Finally, I would like to discuss a 2D example to indicate that well-conditioned fast algorithmic formulations will be applicable even to problems that require volume, as opposed to surface discretization. Given is a 2D problem for which one would like to compute the potential field inside the cavity displayed on the left with the boundary of the volume mesh. The diagram on the right shows the equipotential lines for the computed solution. This problem is extremely difficult to solve using standard methods, both because of the geometric complexity and the unreasonable solution time that would be required. However, using a fast Poisson solver developed using the techniques described here, the time required to solve a problem of arbitrary geometric complexity is only a few times greater than a standard solver using a uniform rectangular mesh on a rectangular domain in which the problem domain can be embedded. Furthermore, the boundary and interior discretizations can be performed totally independently.

Well-conditioned Fast Algorithms

- Orders-of-magnitude faster methods (near-linear computational complexity).
- Prescribable accuracy (well-conditioned matrices) at low cost (easy to design high order schemes).
- Mathematical theory and analytic machinery to reduce computational complexity and memory requirements (sparse matrices).
- Obviate need for complex meshing procedures.

10

Here are the reasons why you should pay attention to harmonic analysis-based methods. Mathematical theory and analytic machinery have been developed over the past ten years that allow the design of orders-of-magnitude faster algorithms, having in most cases near-linear computational complexity. These methods also result in significant memory usage reductions, which is often needed to achieve faster algorithms. The resulting algorithms guarantee prescribable accuracy at low additional cost for additional precision. If that weren't already impressive enough, these schemes involve greatly simplified discretization schemes over those currently required by other methods and should result in an enormous savings to the DoD because of the reduction in time and cost required to discretize complex geometries.

So hopefully, I've piqued your interest in these methods.

Q: When can well-conditioned fast algorithms be developed?

A: Methods are believed to be applicable to most physical problems!

11

Certainly when the underlying physical phenomena are well understood, there is a good chance that well-conditioned fast algorithms can be developed. But as we saw in the space time adaptive processing example, even when the underlying physical process is not initially well understood, the use of representations appropriate to the phenomena can be used not only to derive fast algorithms, but also to shed light on the phenomena themselves.

High-Dimensional Data Exploitation

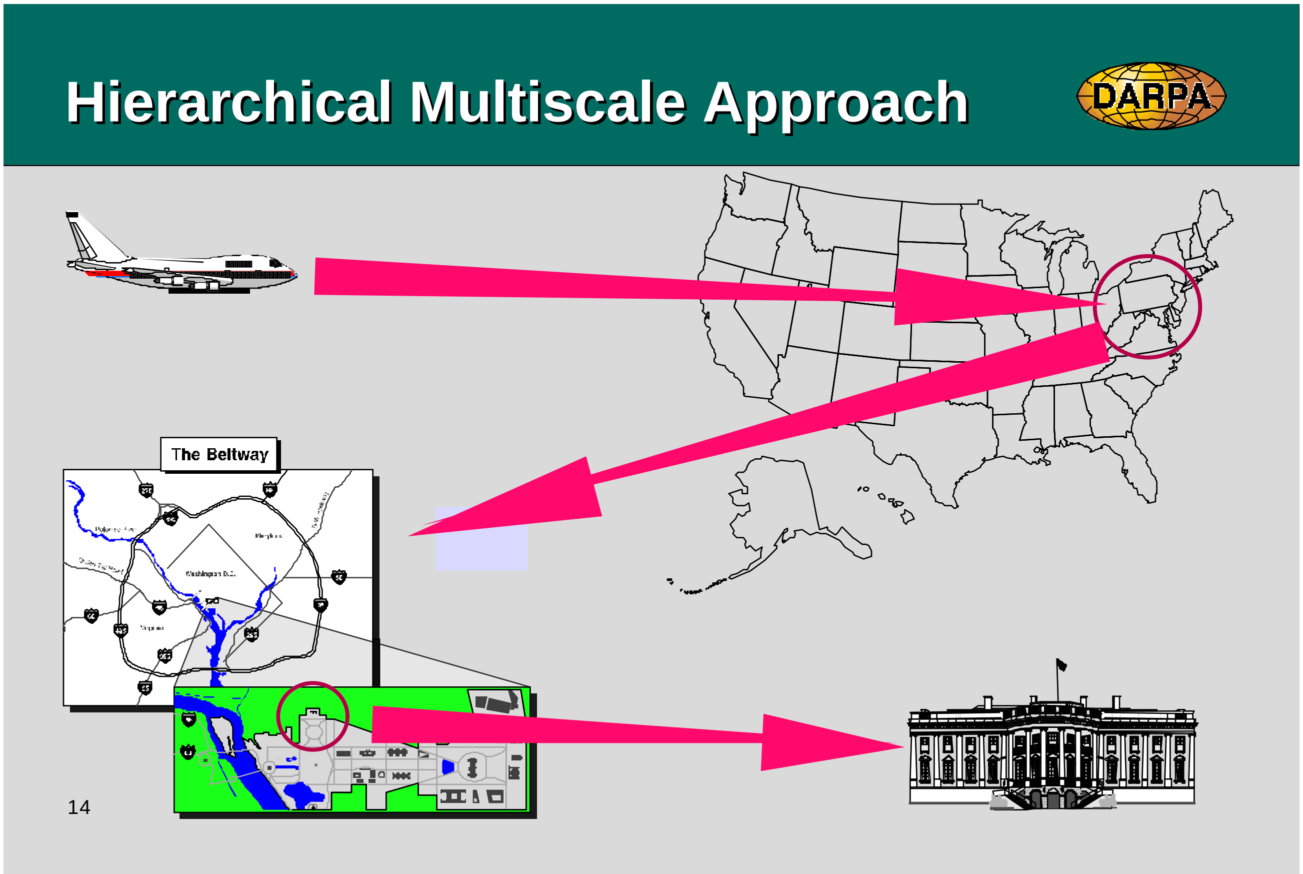
12

Q: What's hard about high-dimensional data?

A: Statistical theory is impractical for large number of degrees of freedom!

13

Much attention in data exploitation problems has been on pattern recognition and statistical methods. But now we are faced with data sets with huge numbers of degrees of freedom to which statistical methods cannot be realistically or correctly applied due to overwhelming data requirements.



This is a notional view of a hierarchical, multiscale approach. When traveling across the country to the East Coast, only coarse geographical information about relative locations of states is needed. Only upon landing in Washington, D.C., does one need more detailed information on major roads to get to the approximate vicinity of the Mall. When one is near the Mall, then one needs even finer information about surface streets and only when one is actually on Pennsylvania Avenue is house number information finally needed to locate the White House. In other words, one zeros in in a hierarchical fashion at successively finer scales. Clearly, just storing all house numbers in the United States is not a winning strategy.

A Proposed Strategy

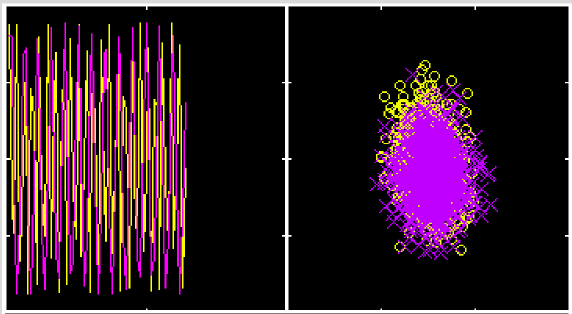
Find hierarchical, multiscale mathematical data representation that

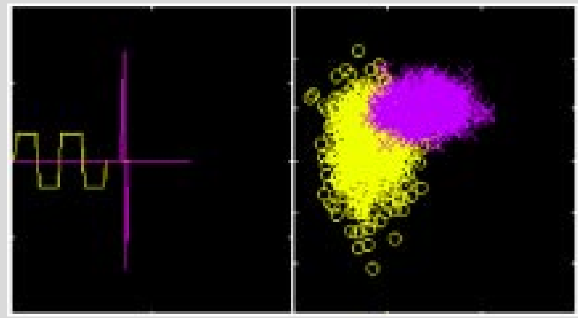
- Is matched to the application (model).
- Allows fast application-specific computer manipulation.
- Allows features of interest to be projected into low-dimensional space.

15

The paradigm of processing in a physically appropriate waveform domain is just as powerful in this problem domain as in the design of well-conditioned fast algorithms. In fact, in automatic target recognition, use of adapted waveform bases of functions such as local trignometric transforms, wavelets, and wavelet packets is based on exactly this paradigm. This methodology is generating considerable interest and excitement because of the ability to efficiently represent coherent information present in signal data. Work to date on development of fast processing schemes using adapted waveform analysis has been extremely promising. The effectiveness of these adapted waveforms lies in their ability to represent complex data in a hierarchical, multiscale fashion. Preliminary indications are that use of these tools should allow dramatic reductions in the required number of degrees of freedom for a broad spectrum of applications.

Longbow Proof-of-Principle Data





Standard Fourier Features ***Best Wavelet Features***

- Over *7%* average classification performance improvement.
- *3.5X* decrease in required computation compared to existing Longbow classifier.

In this slide, using Longbow proof-of-principle data, we give a concrete example of dimensionality reduction enabled by a good representation. In an insertion demonstration project, researchers at Yale University and Lockheed Martin succeeded in designing wavelet-based features that resulted in significant classification improvements over the baseline Longbow Fire Control Radar high resolution ranging system. The plots on the left show the standard Fourier features currently being used to distinguish between two different target classes. In this coordinate system, it is extremely difficult to differentiate between the two targets in any low-dimensional projection. On the other hand, using the two wavelet features shown on the right, a projection can be found that allows reasonably good separation of the targets. This type of processing resulted in an overall classification improvement of over 7% and a 3.5-fold reduction in classification processing required compared to the existing Longbow classifier. The processing throughput gains are due not only to the use of fast wavelet algorithms, but also to the resulting simplifications in the classification algorithms that were enabled by use of a better representation.

Multiscale Representation Possibilities

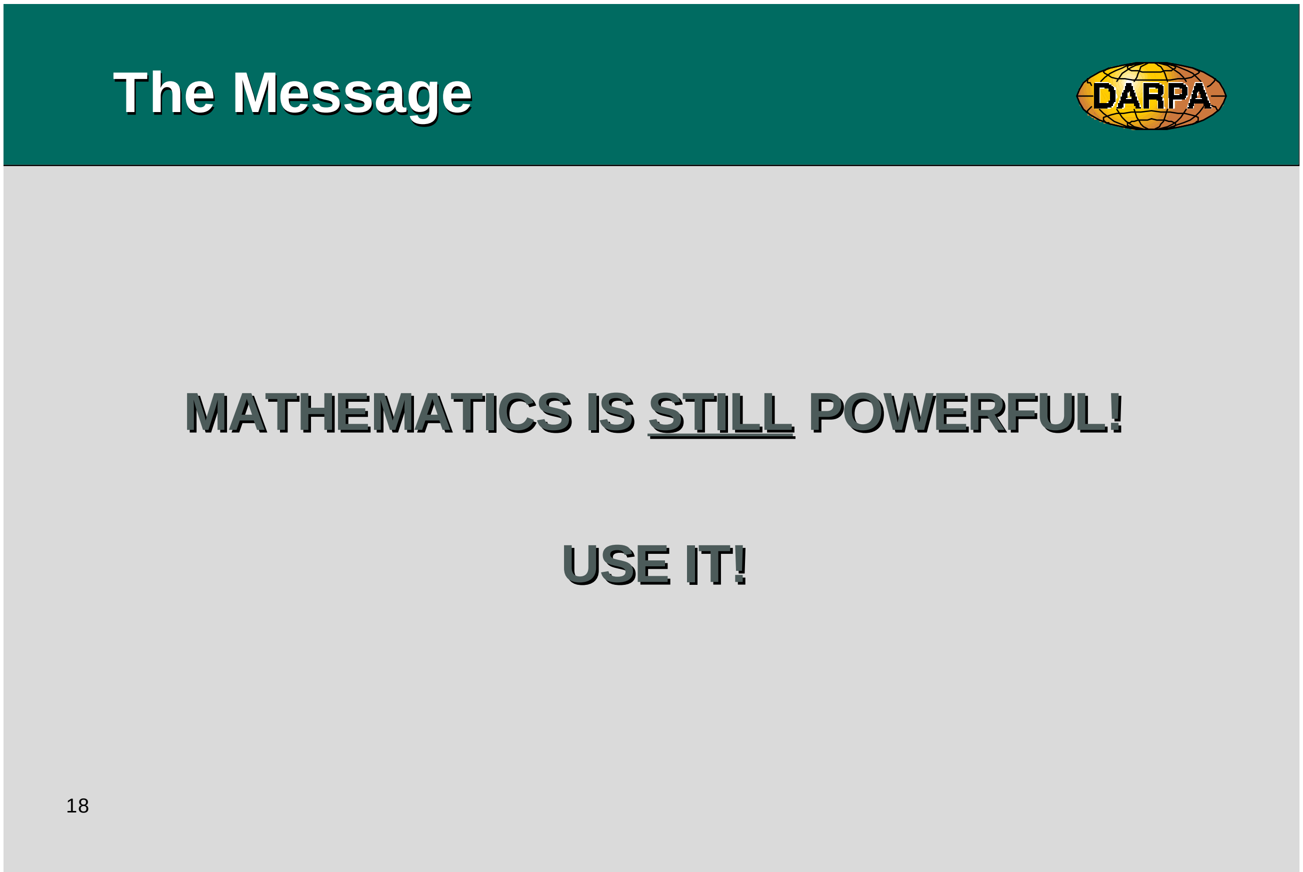
- Bioactivity prediction from molecular structure
  - Long-range electrostatic effects.
  - Binding sites.
  - Local topology.
  - 3D local electrostatic field.
- Digital maps and imagery for strategic/tactical planning
  - Region of world.
  - Country.
  - Topography.
  - Strategically/tactically significant landmarks.

17

The ability to predict biomolecular interactions would be extremely useful in developing strategies to counter biological warfare agents. There is significant potential for harmonic analysis-based methods to improve simulation capability for molecular interactions. In addition, such methods are a much-needed first step in representing 3D molecular structure to allow effective exploitation of the burgeoning data being produced worldwide. Some important application-specific ingredients necessary in hierarchical, multiscale representations of molecular structure are listed.

Harmonic analysis-based methods are undoubtedly also a necessary ingredient in a timely and effective strategy for exploiting digital maps and imagery in military planning.

In both of these applications, as in any signal processing application, an effective representation is only the first step in development of a complete statistical theory for actually mining the data.



Those of you who heard my talk last year may remember my encouragement to use mathematics, since it is powerful. I can’t do any better than to reiterate that message. However, my purpose in alerting you to these particular opportunities is that pulling off the revolution I have described today requires the creativity and focused energy of not just mathematicians, but a broad cross-section of the scientific, computing, and engineering communities. Let’s go to it!